Appendix B

Vadose Zone Modeling

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B-1. Introduction

We performed one-dimensional (1-D) contaminant transport modeling as part of the screening process to determine contaminants of concern in surface and subsurface soil at OUs and release sites at Site 300. The objective of the modeling was to assess the potential impact of residual contaminants present in surface and subsurface soil and rock that could migrate downward through unsaturated sediments (vadose zone) and eventually reach ground water. The results of these simulations are not intended to reflect actual future concentrations at the water table. Instead, these quantitative analyses are intended to represent a conservative worst-case scenario to be used as a screening tool.

Contaminants of potential concern (COPC) in surface and subsurface soil were identified as part of the initial screening process described in Chapter 1, Section 1.3.5. These COPC concentrations were then subjected to both contaminant transport modeling and risk assessment to determine the final contaminants of concern in soil and rock for Site 300. Only those COPCs in soil/rock that present 1) a risk to human health or ecological receptors, and/or 2) a threat to ground water as demonstrated by the 1-D modeling described below, were retained as contaminants of concern.

B-2. Methodology

We began the analyses with identification of known source areas for 1-D vadose zone modeling and the existing contaminants in surface and subsurface soil and/or rock at these sites. We selected sites that have well defined source areas with adequate data to perform a quantitative analysis. We did not model sites that:

- Already have a remedial project in progress [GSA (OU1) and Building 834 (OU2)].
- Have poorly defined source areas [HE Process Area Lagoons and Burn Pit (OU4)].
- Do not have adequate characterization data to perform the analyses (Site 300 OU8; Buildings 812 and 865).
- Have been previously modeled (Site 300 OU8 Building 833 Area).
- Or, are existing landfills (Pits 1, 2, 3, 4, 5, 6, 7, 8, and 9).

After selecting the source areas for 1-D modeling, we selected the COPCs based on the contaminant types, such as metals, radioisotopes and volatile organic compounds (VOCs). To model a reasonable number of COPCs, we used a set of indicator constituents. These COPCs are present in relatively high concentrations/activities, they are widespread, and are representative from a transport-modeling perspective of other similar type COPCs. For example, we used TCE as the indicator constituent to represent all VOCs, since it exists at higher concentrations at the site, and is more mobile from a transport-modeling perspective. We selected beryllium, cadmium, copper, zinc, and lead to represent metals, uranium and tritium to represent radioisotopes, and HMX and RDX to represent high explosive compounds. We also modeled PCBs, dioxins, and furans where they exist in soil/rock.

The following steps are followed when determining impact to ground water from surface and subsurface sediments:

- Develop a representative soil/rock profile for a given source.
- Assign the depth for the ground water table at the bottom of the column.
- Assign the infiltration rate at the top of the column.
- Run the flow portion of the model to determine the soil moisture profile.
- Assign initial contaminant distribution as a profile for contaminated subsurface soils.
- Assign concentrations to the top one-foot of the model for contaminated surface soils.
- Run the transport model and determine elapsed time and maximum concentration/activity reaching the top one-foot of the saturated zone.

B-3. Model Description

We used the numerical code NUFT (**N**onisothermal, **U**nsaturated-Saturated **F**low and **T**ransport Model) (Nitao, 1998) to develop 1-D models representing the unsaturated sediments beneath each source area. NUFT is a multi-phase, multi-component, multi-species flow and transport code that was primarily developed to simulate flow and contaminant transport in the unsaturated and saturated zones. NUFT is capable of simulating all relevant unsaturated and saturated zone processes such as: advection, dispersion, diffusion, adsorption, volatilization, and degradation for aqueous, gaseous, and non-aqueous phases under non-isothermal conditions.

We did not select other 1-D screening models such as VLEACH and SESOIL as our tool of analysis because of limiting assumptions embedded in these codes. The limiting assumptions are mainly the homogenous soil properties, constant soil moisture profiles, and the definition of several constitutive relationships. Using a homogenous soil profile is not suitable for Site 300 source areas since the geology is very complex and we observe different lithologies ranging from coarse artificial fill materials to very fine bedrock in the source areas. Assuming a constant soil moisture profile is not representative since we observe distinct changes in soil moisture with depth, corresponding to the heterogeneous soil profiles. We also observe distinct changes in relative permeability, soil moisture retention characteristics, and adsorptive properties for these heterogeneous soil types.

B-4. Conceptual Model

B-4.1. Input Parameter Estimation

We used soil/rock boring logs and remedial investigation results to characterize the geology and develop representative conceptual models for each source area. For transport modeling purposes, we used a conservative approach when determining sediment properties, model structure, and contaminant properties. We considered two pathways originating from residual contaminants: contaminants in subsurface soils and surface soils migrating downward to the water table. Summarized below are the primary methodologies we used during development of site models and the selection of input parameters.

B-4.1.1. Soil/rock Profiles

We developed lithologic profiles based on well logs from borings/wells in the vicinity of the source areas. We used an interpretation of these profiles that has conservative contaminant transport characteristics. For example, we disregarded fine soil/rock layers that were not consistently present in borings throughout the source area, and chose to representative high-permeable layers using the maximum thickness encountered and adjacent low-permeability layers using the minimum thickness encountered. For firing tables, we combined the firing table profile with the subsurface profile to create one continuous lithologic profile. Table B-1 describes the sources of information we used to determine the lithologic profile for each source area.

Once we established a lithologic profile, we then translated it into a soil/rock profile containing materials from any of six categories. We discuss the properties of these six categories below. The resulting soil/rock NUFT profiles are described in detail in the modeling report (Demir et. al., 1998).

B-4.1.2. Unsaturated Zone Thickness

We assumed a conservative unsaturated zone thickness for each model based on highest historical ground water elevations, which result in thinnest unsaturated zone thickness. When confined zones were encountered, we selected the top of the saturated sediments to be the target ground water elevation, since this is the depth for contaminants to travel to reach ground water.

B-4.1.3. Hydraulic Properties

We divided the unsaturated sediments underlying the source areas into six physical property categories. These soil/rock types are: (1) coarse artificial fill material, (2) fine artificial fill material, (3) coarse soils, (4) fine soils, (5) coarse bedrock, and (6) fine bedrock. This grouping is developed by a review of soil samples from 23 locations at Site 300 that were analyzed for their unsaturated hydraulic and moisture retention properties (Demir et. al., 1999). When we plotted characteristic property curves together from these samples, we observed three major groups: Materials that can be defined as artificial fill materials, soils, and bedrock. We further refined this grouping by the range of values, or the envelopes defining these groups. The minimum and maximum values in these ranges represent finer sediments and coarser sediments for that group. For each of the six soil/rock groups we selected representative soil/rock properties within these ranges, and used them as input values in the NUFT modeling. Care was taken to conservatively select higher permeability, porosity, and moisture content parameter values to represent each group.

B-4.1.4. Infiltration Rate

To conservatively estimate a worst-case infiltration rate for Site 300 source areas, we conducted a water balance analysis. We used daily precipitation data and other climatic data together with surface properties, such as sediment types and hill slopes. As a result of this sensitivity study (Demir et. al., 1999), we selected an infiltration rate of 6 in/yr (approximately 16 cm/yr), to be the conservative infiltration rate. This rate is equivalent to 50% of average annual rainfall (12.6 in/yr). This high infiltration rate together with the conceptual model, which does not consider evapotranspiration and volatilization, yields very conservative input values resulting in constant downward flux of contaminants. In effect, this represents repetitive years of heavy rainfall.

B-4.1.5. Transport Parameters

We selected partitioning coefficients for each COPC to be the smallest reported literature values. A small liquid/solid partitioning coefficient means less sorptive (more mobile) constituents. A small (essentially negligible) liquid/air partitioning coefficient means non-volatile constituents. This selection conservatively estimates the maximum concentration of constituents that can potentially reach ground water. We did not use dispersivity in the models, in effect creating a plug-flux model of constituents reaching the ground water at the maximum possible peak concentration.

B-4.2. Model Initialization and Boundary Conditions

Prior to modeling the transport of constituents from unsaturated soil/rock to ground water, we calibrated each model to existing initial moisture content distributions for sites where data were available. The Building 850 firing table area has the most representative data set; therefore we used this site to calibrate the input parameters for sediment types to match the soil moisture profile. We conservatively shifted the moisture profiles towards a wetter profile to account for extended duration of heavy rainfall. Once we calibrated soil properties to this data set, the soil moisture profiles of other sites closely represented their actual field conditions based on their lithological descriptions.

We conservatively ignored dilution due to ground water flow in the models. Concentration values reported for each constituent represents the maximum value that reaches the top one-foot of the saturated zone. Assuming a simple box-model to account for the mixing, and assuming conservative ground water flow properties typical to Site 300, the maximum reported values could be conservatively reduced by 30% to 50% due to ground water dilution.

We assigned initial soil/rock concentrations to the model according to the following method: for COPCs that were observed to depths greater than one foot, we developed a conservative soil/rock concentration profile by averaging only detected values from all surrounding boreholes. To determine impact to ground water from surface soils, we assigned the highest measured concentration at or near the source area to the top one foot of the model.

B-5. Conclusions

Simulation results are displayed in Table B-2. We present the highest concentration to reach the ground water and the arrival time along with background and MCL concentrations for comparison. The COPCs that are presented in the last column of Table B-2 impact ground water under a worst-case scenario. The remaining COPCs, under conservative vadose zone modeling show no impact to ground water. The COPCs that generally do not impact the ground water have either very high adsorption properties and do not migrate down to ground water (PCBs, dioxins, HMX, and some metals), or they are radioisotopes with short half-lives (tritium). The COPCs that indicate impact to ground water under these conservative screening level modeling assumptions may not necessarily reach the ground water. The results also indicate impact levels in some source areas that are higher than existing ground water concentration levels. This is an indication of the level of conservatism that was employed for the current analysis. Further detailed quantitative analysis is required to assess the realistic potential impact of these contaminants to ground water under site-specific conditions.

B-6. References

Demir, Z., and L. Ferry (1999) Assessment of impact to ground water from vadose zone sources for the Site 300 Site-Wide Feasibility Study, Lawrence Livermore National Laboratory, Calif. (UCRL-AR-135312).

Nitao, J. (1998), User's Manual for the UNST module of the NUFT code, version 2.0 (NP-phase, NC-component, thermal), Lawrence Livermore National Laboratory, Calif. (UCRL-MA-130653).

Table B-1. Soil/rock profile and ground water elevation information sources for NUFT modeling.

Location	Source of soil/rock profile and ground water elevation information
HE Process Area - Building 815	Lithologic descriptions from nearby wells W-815-01 and -02. Unconfined and confined ground water elevations from wells W-815-01 and -02.
Building 850 Firing Table	Lithologic descriptions from nearby wells NC7-44, NC7-70, and borings B-850-01 through -04. Unconfined ground water elevation inferred from upgradient well NC7-44 and down gradient well NC7-70.
Building 854 Complex	Lithologic descriptions and unconfined ground water elevation from nearby well W-854-02.
Building 832 Complex	Lithologic descriptions and unconfined ground water elevation from nearby wells W-832-12 through -21.
Building 830 Complex	Building 832 Canyon Complex soil/rock profile and unconfined ground water elevation were used. These two sites have essentially the same characteristics.
Building 801D Dry Well	Lithologic descriptions from nearby wells K8-01 and -03B. Unconfined ground water elevation inferred from upgradient well NC2-13 and down gradient well K8-03B.
Building 802 Firing Table	Lithologic descriptions from nearby well NC2-05A and from nearby borings B-802-01 through -04. Potentiometric surface from well NC2-05, and top of the confined aquifer was selected as the target ground water elevation.
Building 845 Firing Table	Lithologic descriptions from nearby well K9-01, and borings B-845-01 through -04. Unconfined ground water elevation from well K9-01.
Building 851 Firing Table	Lithologic descriptions from nearby wells W-851-05 through -08, and borings B-851 through -05. Unconfined ground water elevation from wells W-851-05, -06, and -07.

Table B-2. NUFT modeling results.

Location	Contaminant of Concern	Maximum concentration /activity to reach ground water	Time for Maximum concentration /activity to reach ground water (years)	Background concentration /activity	MCL for ground water	Units	Potential impact to ground water above background levels
Subsurface sources							
HE Process Area							
Perched horizon	TCE	216	50	0.5[a]	5.0E+00	µg/L	Yes
	HMX	580	500	–	1.8E+00[c]	mg/L	Yes[b]
Bedrock Aquifer	TCE	154	130	0.5[a]	5.0E+00	µg/L	Yes
Building 850 Firing Table							
	Tritium	1.3E+06	7	300	2.0E+04	pCi/L	Yes
	Uranium-total	180	700	0.121	2.0E+01	pCi/L	Yes
Building 854 Complex							
	TCE	600	300	0.5[a]	5.0E+00	µg/L	Yes
Building 832 Complex							
	Tritium	300	10	300	2.0E+04	pCi/L	No
	HMX	0.13	50	–	1.8E+00[c]	mg/L	Yes[b]
Building 830 Complex							
	Tritium	200	10	300	2.0E+04	pCi/L	No
Building 801D Dry Well							
	TCE	15	200	0.5[a]	5.0E+00	µg/L	Yes
Building 802 Firing Table							
	Tritium	240	30	300	2.0E+04	pCi/L	No

Table B-2. NUFT Modeling Results. (Cont. Page 2 of 4)

Location	Contaminant of Concern	Maximum concentration /activity to reach ground water	Time for Maximum concentration /activity to reach ground water (years)	Background concentration /activity	MCL for ground water	Units	Potential impact to ground water above background levels
Building 845 Firing Table							
	Tritium	200	40	300	2.0E+04	pCi/L	No
	Uranium-total	42	2.75E+03	0.121	2.0E+01	pCi/L	Yes
	HMX	0.014	260	–	1.8E+00[c]	mg/L	Yes[b]
Building 851 Firing Table							
	Uranium-total	786	4.6E+03	0.121	2.0E+01	pCi/L	Yes
Surface soil sources							
Building 850 Firing Table and surrounding area							
	Beryllium	0.0049	2.0E+04	0.004	4.0E-03	mg/L	No
	Cadmium	0.0194	3.3E+03	0.0015	5.0E-03	mg/L	Yes
	Copper	1.75	3.0E+03	0.05	1.0E+06[c]	mg/L	Yes[b]
	Tritium	190	20	300	2.0E+04	pCi/L	No
	Uranium-total	460	820	0.121	2.0E+01	pCi/L	Yes
	Dioxin (2,3,7,8-TCDD)	4.0E-09	3.0E+06	0.001[a]	3.0E-05	µg/L	No
	Furans	0.002	4.0E+03	0.001[a]	6.1E+00[c]	µg/L	Yes[b]
	PCBs	0.036	1.5E+07	0.5[a]	5.0E-01	µg/L	No

Table B-2. NUFT Modeling Results. (Cont. Page 3 of 4)

Location	Contaminant of Concern	Maximum concentration /activity to reach ground water	Time for Maximum concentration /activity to reach ground water (years)	Background concentration /activity	MCL for ground water	Units	Potential impact to ground water above background levels
Building 854 Complex							
	Cadmium	0.00094	2.0E+04	0.0015	5.0E-03	mg/L	
	Lead	1.9	2.0E+05	0.02	1.5E+01[e]	µg/L	Yes[b]
	Uranium-238	1.3	5.0E+03	0.121	2.0E+01[f]	pCi/L	Yes[b]
	HMX	1.7	500	–	1.8E+00[c]	mg/L	Yes[b]
	PCBs	0.0015	8.0E+07	0.5[a]	5.0E-01	µg/L	No
Building 802 Firing Table and surrounding area							
	Tritium	0.08	30	300	2.0E+04	pCi/L	No
	Uranium-total	41.0	2.0E+03	0.121	2.0E+01	pCi/L	Yes
Building 845 Firing Table and surrounding area							
	Tritium	0.4	40	300	2.0E+04	pCi/L	No
Building 851 Firing Table and surrounding area							
	Beryllium	2.3E-05	2.0E+04	0.004	4.0E-03	mg/L	No
	Cadmium	0.0024	2.0E+04	0.0015	5.0E-03	mg/L	Yes[b]
	Copper	0.054	2.0E+04	0.05	1.0E+06[c]	mg/L	Yes[b]
	Zinc	0.041	1.0E+04	0.01	5.0E+00[c]	mg/L	Yes[b]
	Tritium	0.6	70	300	2.0E+04	pCi/L	No

Table B-2. NUFT Modeling Results. (Cont. Page 4 of 4)

Location	Contaminant of Concern	Maximum concentration /activity to reach ground water	Time for Maximum concentration /activity to reach ground water (years)	Background concentration /activity	MCL for ground water	Units	Potential impact to ground water above background levels
Building 851 Firing Table and surrounding area (cont.)							
	Uranium-total	24.0	5.0E+03	0.121	2.0E+01	pCi/L	Yes
	RDX	2.5	400	0.7[a]	6.1E-01[b]	µg/L	Yes

[a] **Reporting limit.**

[b] **Concentration or activity in ground water below MCL or PRG.**

[c] **PRG.**

[d] **Secondary MCL.**

[e] **Action level.**

[f] **MCL for total uranium.**